

4-Phenyltoluene
644-08-6 | DTXSID4047177

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1980 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.19e-01

Confidence level: 8.30e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Diphenyl oxide</div> <div>Measured: 1950</div> <div>Predicted: 1170</div>	<div>Image not found</div> <div>2-Ethyl-naphthalene</div> <div>Measured: 5750</div> <div>Predicted: 3850</div>	<div>Image not found</div> <div>Benzophenone</div> <div>Measured: 427</div> <div>Predicted: 415</div>
<div>Image not found</div> <div>Biphenyl</div> <div>Measured: 1860</div> <div>Predicted: 2430</div>	<div>Image not found</div> <div>2-Chlorobiphenyl</div> <div>Measured: 2950</div> <div>Predicted: 3250</div>	